

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -65.0 °C

Global applicability domain: Inside

Local applicability domain index: 7.05e-01

Confidence level: 4.95e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Allyl alcohol</div> <div>Measured: -129</div> <div>Predicted: -109</div>	<div>Image not found</div> <div>1-Butanol</div> <div>Measured: -89.8</div> <div>Predicted: -95.0</div>	<div>Image not found</div> <div>1-Propanol</div> <div>Measured: -126</div> <div>Predicted: -114</div>
<div>Image not found</div> <div>Hexa-2,4-dien-1-ol</div> <div>Measured: 30.5</div> <div>Predicted: 1.05</div>	<div>Image not found</div> <div>(2E,4E)-Hexa-2,4-dien-1-ol</div> <div>Measured: 30.5</div> <div>Predicted: 1.05</div>	<div>Image not found</div> <div>2-Butyn-1-ol</div> <div>Measured: -2.20</div> <div>Predicted: -25.1</div>